

Please amend the application, without prejudice, in accordance with the following.

In the Claims:

Re-write the claims as follows:

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4. (Amended) The method as claimed in [either of claims 2 or 3] claim 2, wherein the total data in the reduced representation is reduced by a factor substantially equal to the number of data points in the original powder diffraction data divided by the number Bragg reflections in the measured data range.

5. (Amended) The method as claimed in [either of claims 3 or 4] claim 3, wherein the fitness χ^2 of each of the trial structures is determined using the following function:

$$\chi^2 = \sum_b \sum_k \{(I_b - c |F_b|^2) (V^{-1})_{bk} (I_k - c |F_k|^2)\}$$

where:

$I_{h,k}$ = extracted intensity

$V_{h,k}$ = covariance matrix

c = a scale factor

$F_{h,k}$ = calculated structure factor from trial structure

6. (Amended) The method as claimed in [any one of the preceding claims] claim 1, wherein the set of variables consists of three coordinates representative of the location of the molecule within the unit cell and three independent coordinates representative of the orientation of the molecule within the unit cell.

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8. (Amended) The method as claimed in [any one of the preceding claims] claim 1 including the step of determining the unit cell and space group for the molecule under examination.

9. (Amended) The method as claimed in [any one of the preceding claims] claim 1 including the step of determining the set of internal coordinates.

*A²
Concl'd.*

10. (Amended) The method as claimed in [any one of the preceding claims] claim 1, further including the step of monitoring the number of iterations in which new trial structures are generated and halting the method and outputting the trial crystal structure with the best calculated fitness after completion of a predetermined number of iterations.

11. (Amended) The method as claimed in [any one of the preceding claims] claim 1, wherein the selection of survivors and the alteration of the values of the variables is based on a simulated annealing procedure.

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15. (Amended) The method as claimed in [either of claims 13 or 14] claim 13, wherein the total data in the reduced representation is reduced by a factor substantially equal to the number of data points in the original powder diffraction data divided by the number Bragg reflections in the measured data range.

16. (Amended) Apparatus as claimed in [either of claims 14 or 15] claim 14, wherein the fitness analyser determines the fitness χ^2 of each of the trial structures using the following function:

$$\chi^2 = \sum_b \sum_k \{(I_b - c |F_b|^2) (V^{-1})_{bk} (I_k - c |F_k|^2)\}$$

where:

$I_{h,k}$ = extracted intensity from the structure factor analyser

$V_{h,k}$ = covariance matrix from the structure factor analyser

c = a scale factor

$F_{h,k}$ = calculated structure factor from trial structure

17. (Amended) Apparatus as claimed in [any one of claims 12 to 16] claim 12, wherein controller determines a set of variables consists of three coordinates representative of the location of the molecule within the unit cell and three independent coordinates representative of the orientation of the molecule within the unit.